Methodologies for Scale-bridging in Multi-scale Simulation

S&T Campaign: Computational Sciences
Predictive Simulation Sciences

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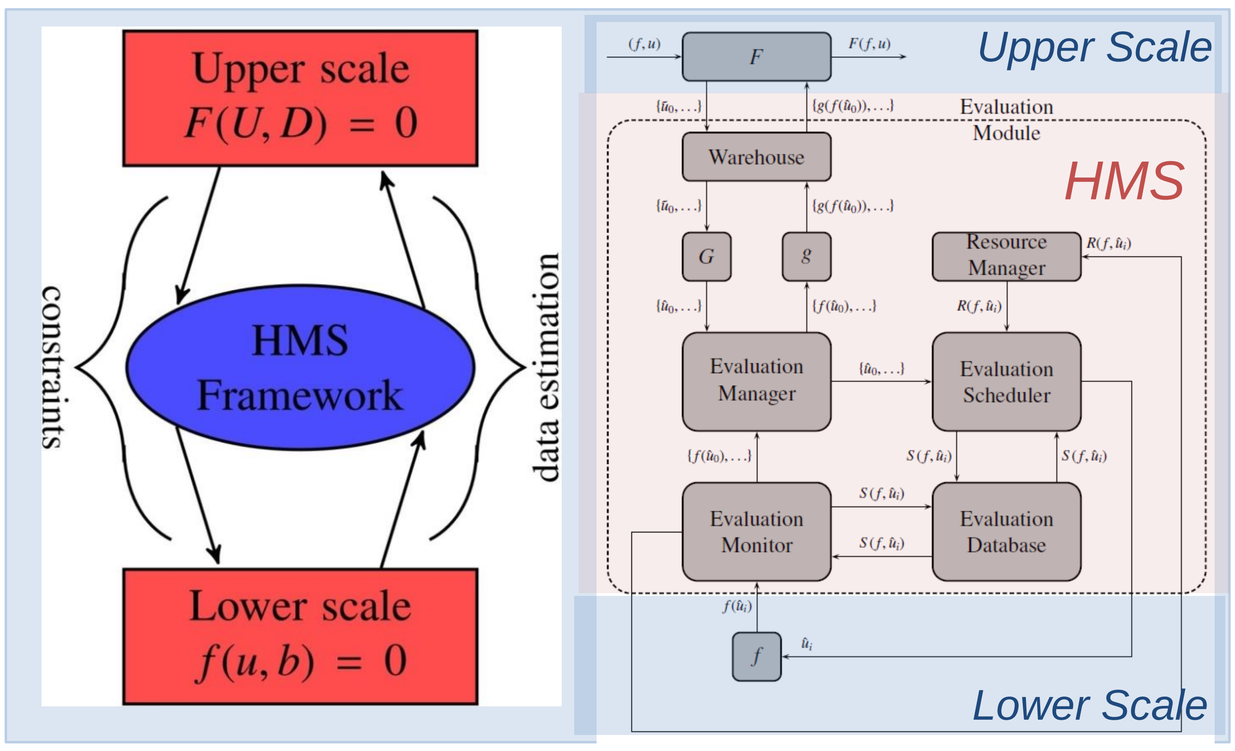
Research Objective

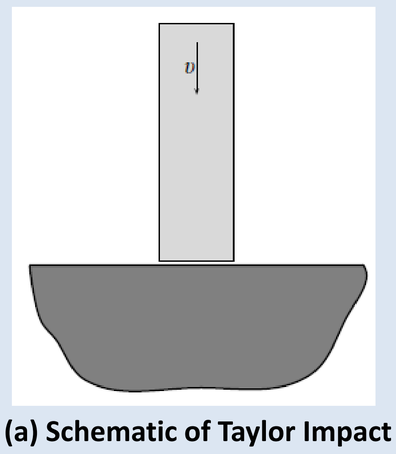
- **Develop numerical and computational methodologies for scale-bridging in hierarchical (sequential and concurrent) multi-scale simulations of materials on extreme scale computing platforms**



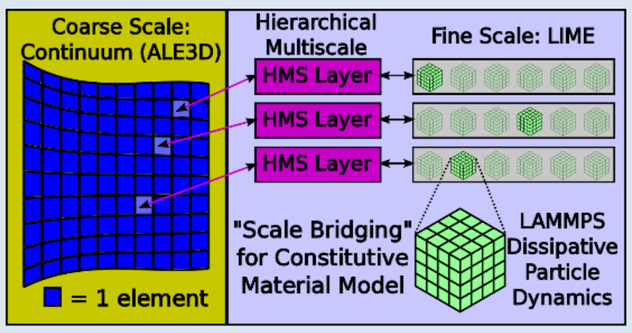
Two-scale hierarchical model.

Challenges

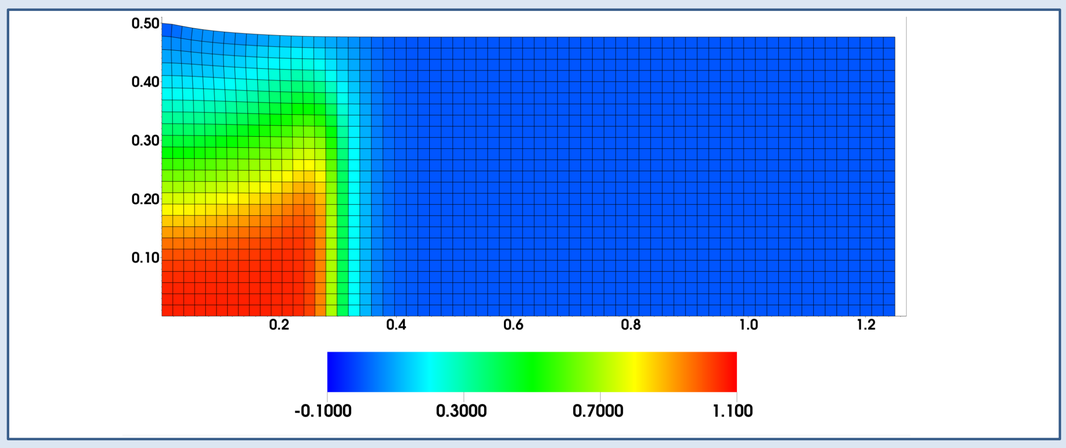
- **Development of new multi-scale models is severely hindered by the lack of general numerical and computational methodologies for scale-bridging**
- **Multi-scale material model hierarchy is usually adaptive and highly dynamic. However, current parallel computing environments remain static and lack support for adaption**



(a) Schematic of Taylor Impact Experiment



(b) Two-scale hierarchy incorporating dissipative particle dynamics

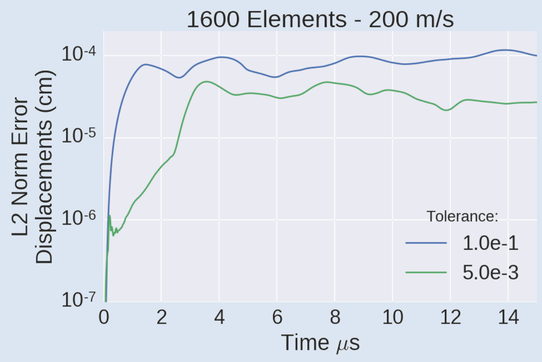


(c) Pressure at 1.0 us for 1600 element macroscopic model

Taylor impact simulation of an energetic material.

ARL Facilities and Capabilities Available to Support Collaborative Research

- **Developed numerical methodologies, proof-of-concept implementation of scale-bridging framework (HMS) and utilized it to construct multi-scale applications for electrochemistry, energetic materials, and bone surrogate materials**
- **Numerical techniques for adaptive generation of multi-fidelity surrogate-models under development**
- **Managing highly dynamic hierarchies, especially load-balancing and fault-tolerance, is critical to achieving practical multi-scale applications**
- **Incorporation of surrogate models through methods such as adaptive sampling (kriging) is necessary to alleviate computational cost, but may also exacerbate load imbalance**



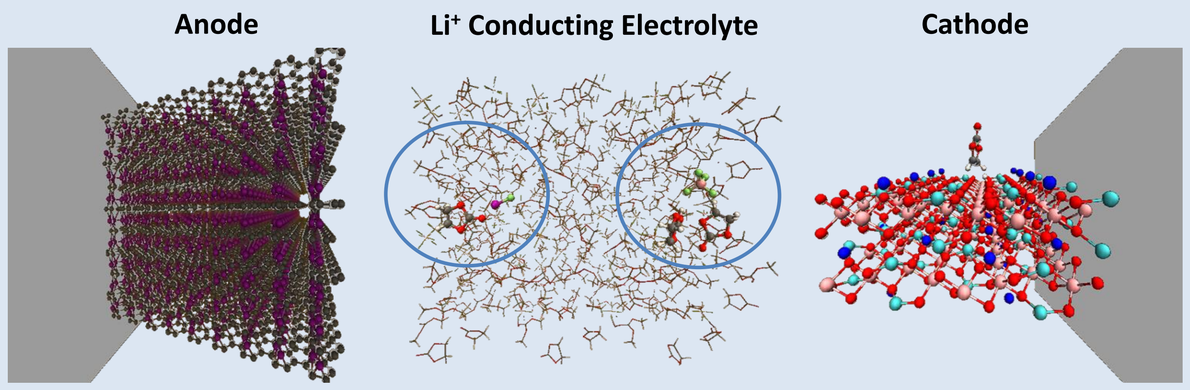
(a) L_2 error of solution for different adaptive sampling tolerances

(b) Interpolation rate for different adaptive sampling tolerances

Adaptive Surrogate Modeling for Multiscale Simulation

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- **New methods and algorithms for time-dependent lower scale models**
- **Methods for interpolation in high-dimensional spaces.**
- **Surrogate modeling techniques**
- **Data estimation and analytics related to microscopic model response (e.g. time evolution and reconstruction of microstructure)**
- **Validation of our scale-bridging methodologies**
- **Uncertainty quantification**



HMS driving exploration of novel battery chemistries